CSI 436/536
Introduction to Machine Learning

SVM algorithm

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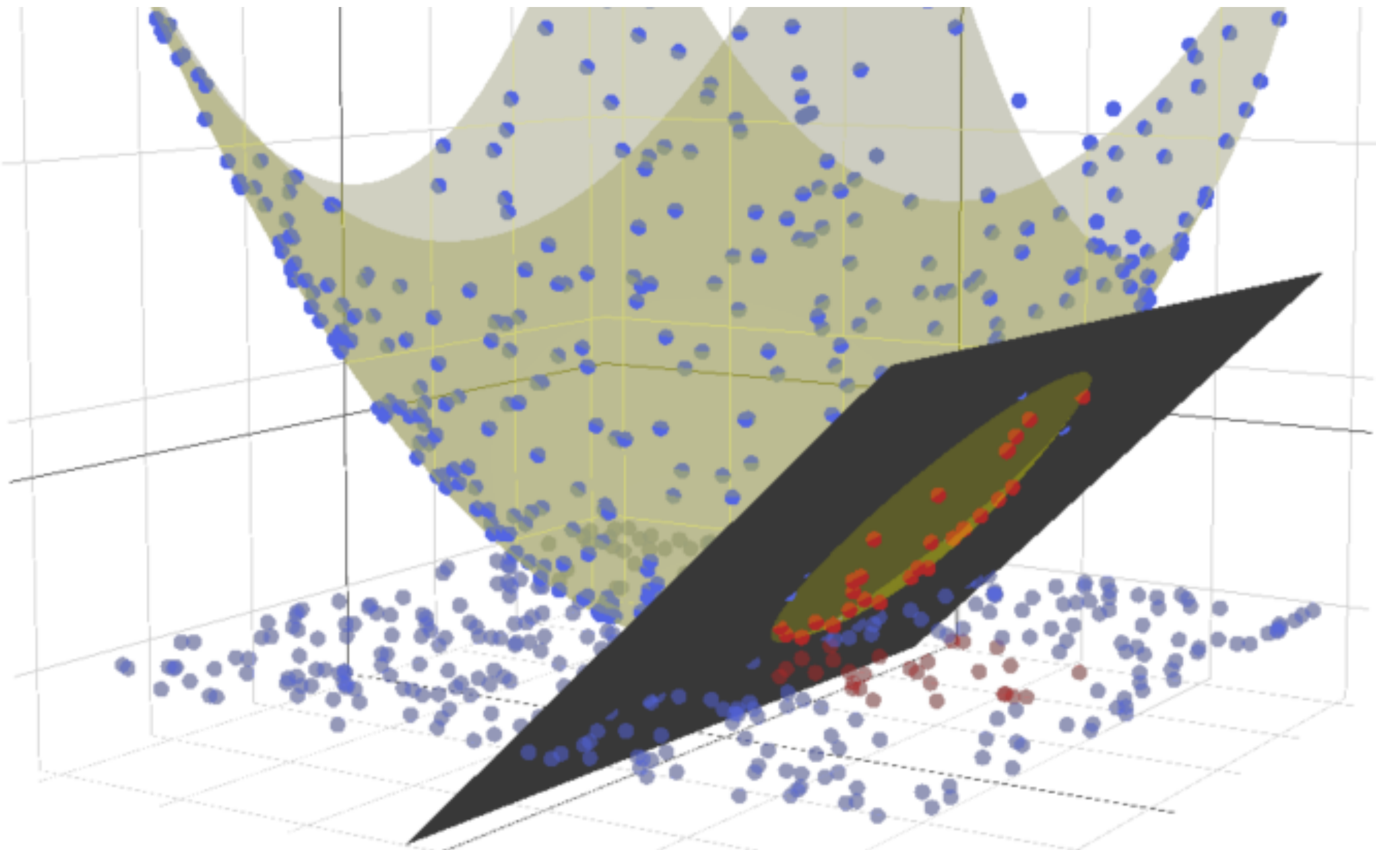
Solving SVM: separable case

- SVM in separable case is to

$$\text{Minimize } ||w||^2, \quad \text{subject to: } y_i(w \cdot x_i + b) \geq 1$$

- How do we solve this quadratic programming problem numerically?



constrained optimization

- to solve $\min_x f(x)$ s.t., $g(x) \leq 0$
  - general idea: convert to unconstrained problem
  - three types of general methods
    - the barrier method, e.g.,
      $\min_x f(x) + \log(-g(x))$: always feasible
    - the penalty method, e.g.,
      $\min_x f(x) + \max(0, g(x))$: can be infeasible
    - primal-dual method, using Lagrangian duality

constrained optimization

- Lagrangian and Lagrangian multipliers for the primal problem

  $$\min_x f(x) \text{ s.t., } g(x) \leq 0$$

  - introduce multiplier $0 \leq \lambda$ and form Lagrangian

    $$L(x, \lambda) = f(x) + \lambda g(x)$$

  - for any feasible x, $L(x,\lambda) \leq f(x)$, i.e., a lower bound

- dual problem
  - first, find $x^*(\lambda) = \text{argmin}_x L(x,\lambda)$
  - dual function: $h(\lambda) = L(x^*(\lambda),\lambda)$ is concave
  - $\max_\lambda h(\lambda)$, s.t., $0 \leq \lambda$ is the dual problem

weak & strong duality

- f^* = optimal value of the primal problem

  $$\min_x f(x) \text{ s.t., } g(x) \leq 0$$

- h^* = optimal value of the dual problem

  $$\max_\lambda h(\lambda), \text{ s.t., } 0 \leq \lambda$$

- with very loose conditions, we always have

  $$h^* \leq f^*$$

  this is known as the weak duality

- with more assumptions (e.g., primal problem is convex), we have

  $$h^* = f^*$$

  this is known as the strong duality

- many problem can be solved easily in the dual form

KKT condition

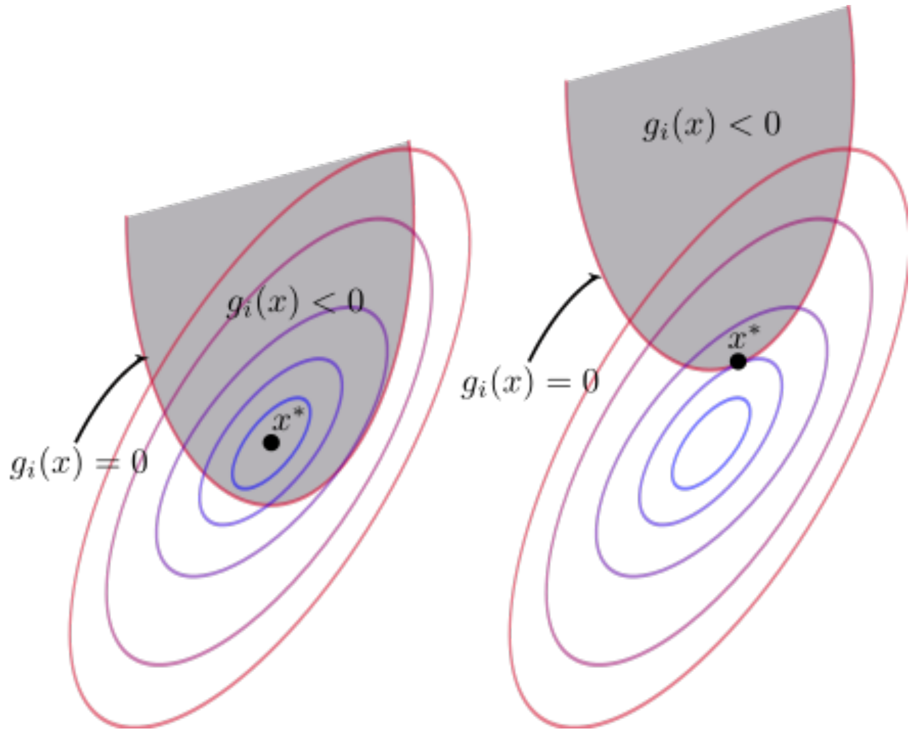
- Karush-Kuhn-Tucker condition
  - gradient of Lagrangian has to be zero

    $$\nabla f(x) + \lambda \nabla g(x) = 0$$

  - primal feasibility: $g(x) \leq 0$
  - dual feasibility: $\lambda \geq 0$
  - complementary slackness: $\lambda g(x) = 0$
- counterpart of the optimal condition of $\nabla f(x) = 0$ for unconstrained optimization

understanding the KKT condition

- Two cases



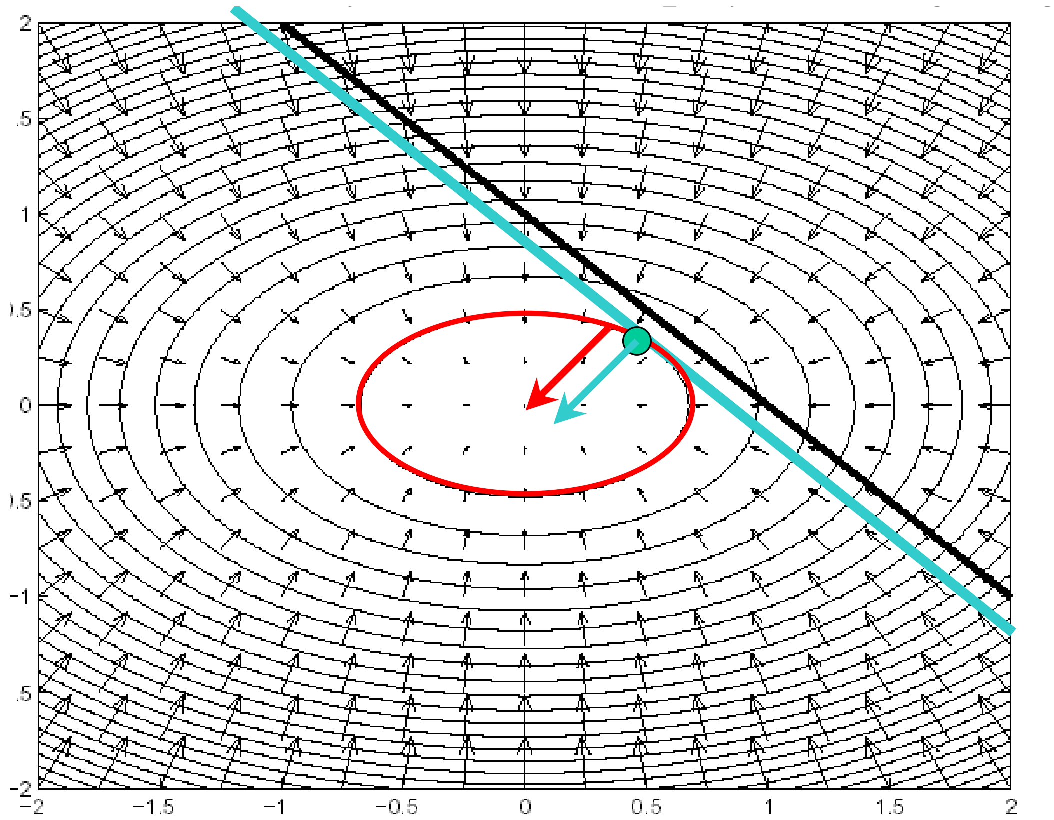
  - Case 1: optimal solution inside feasible region
    $\nabla f(x) = 0, \lambda = 0, g(x) < 0$
  - Case 2: optimal solution on boundary
    $\nabla f(x) \propto -\nabla g(x), \lambda > 0, g(x) = 0$

understanding the KKT condition

- optimal solution
  - inside the feasible region
    - gradient of objective function is zero
  - on the boundary of the feasible region
    - gradient of objective function is orthogonal to the linear constraint form the boundary
- which case is indicated by the Lagrangian multiplier $\lambda \geq 0$
  - $\lambda = 0$: inside feasible region
  - $\lambda > 0$: on the boundary of feasible region

Example

- $\min_{x,y} f(x,y) = x^2+2y^2$, s.t., $x+y \geq 1$



solving SVM: separable case

Primary problem

$$\min_{\mathbf{w},\mathbf{b}} \frac{1}{2}\|\mathbf{w}\|^2$$
$$\text{s.t.} \quad y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 \text{ for } i = 1, \cdots, n$$

Introducing multipliers $\alpha_i \geq 0$ and forming Lagrangian

$$L(\mathbf{w}, b, \alpha) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{n} \alpha_i y_i(\mathbf{w}^T\mathbf{x}_i + b) + \sum_{i=1}^{n} \alpha_i.$$

solving SVM: separable case

- We can solve the primary problem directly
  - Solution always exist when data are separable
  - But some elegant geometry is buried in the solution
- We instead solve the dual problem after removing primal variables because
  - KKT condition requires many multipliers to take zero values
  - training examples whose corresponding multiplier take nonzero values are the **support vectors**

solving SVM: separable case

Eliminate primal variables **w** and b

$$\begin{aligned}\frac{\partial L(\mathbf{w}, b, \boldsymbol{\alpha})}{\partial \mathbf{w}} &= \mathbf{w} - \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = 0 \\ \frac{\partial L(\mathbf{w}, b, \boldsymbol{\alpha})}{\partial b} &= \sum_{i=1}^{n} \alpha_i y_i = 0\end{aligned}$$

From the first condition, we have $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$.

From the second condition, we have $\sum_{i=1}^{n} \alpha_i y_i = 0$.

Complementary slackness (from KKT condition)

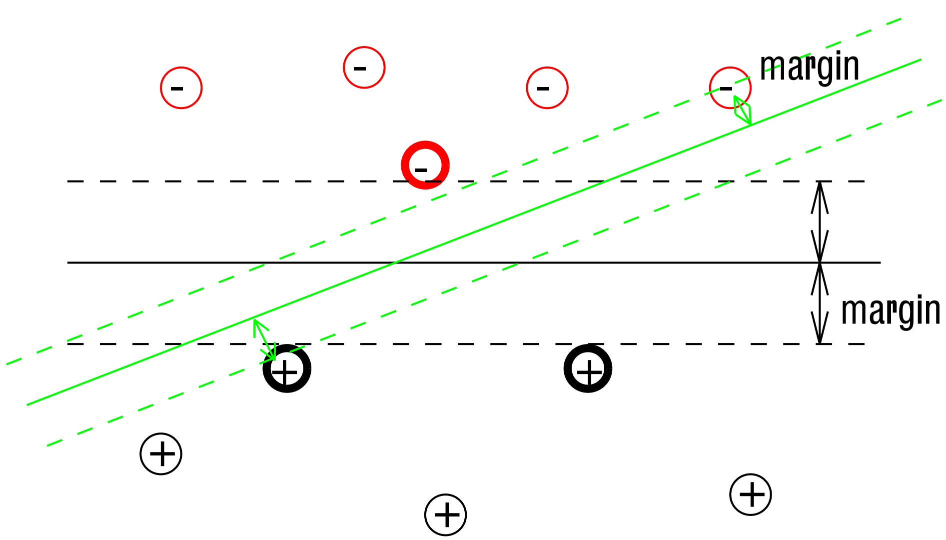
$\alpha_i(y_i(\mathbf{w}^T\mathbf{x}_i + b) - 1) = 0$.

solving SVM: separable case

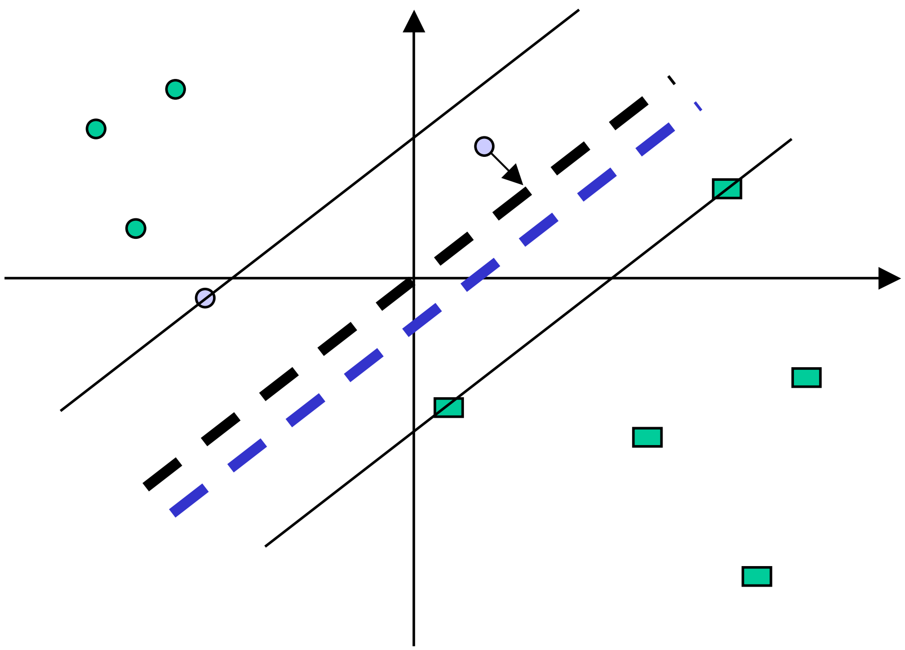
Eliminate primal variables **w** and b with $\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$ and $\sum_{i=1}^{n} \alpha_i y_i = 0$, the dual problem becomes

$$\max_{\boldsymbol{\alpha}} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

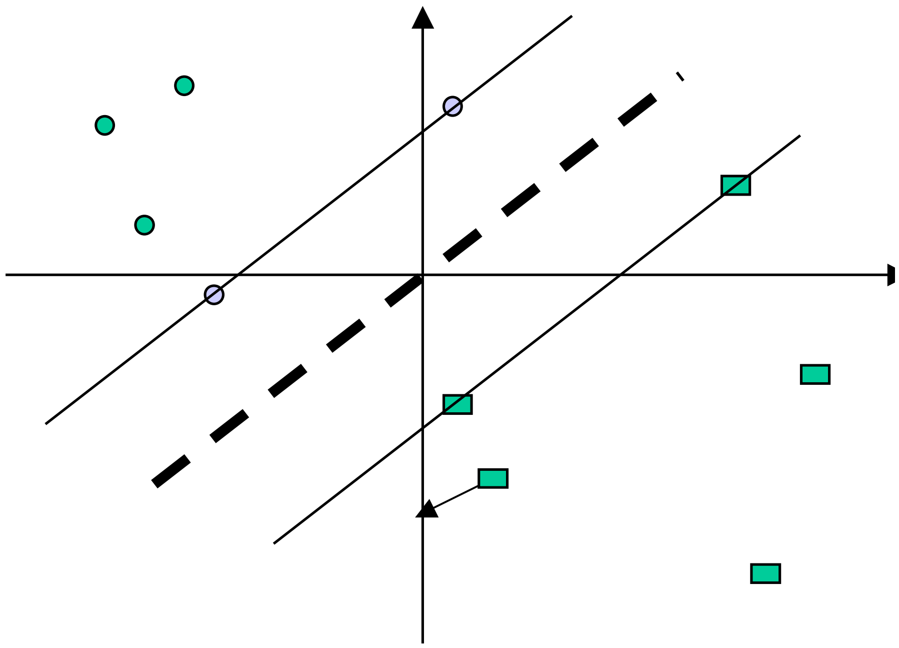
$$\text{s.t.} \quad \sum_{i=1}^{n} \alpha_i y_i = 0, \alpha_i \geq 0.$$



Support vectors



Moving a support vector moves the decision boundary



Moving the other vectors has no effect

solving SVM: non-separable case

Minimize:

$$||w||^2 + C\sum_{i=1}^{m}\xi_i$$

subject to:

$$y_i(w \cdot x_i + b) \geq 1 - \xi_i, \quad \xi_i \geq 0$$

Dual form:

$$\max_{\alpha} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{s.t.} \quad \sum_{i=1}^{n} \alpha_i y_i = 0, \; 0 \leq \alpha_i \leq C$$

Solving SVM

- The quadratic programming problem for either separable and non-separable cases can be solve efficiently using off-the-shelf packages
- We introduce however a particularly simple optimization scheme known as sequential minimization optimization (SMO) based on the paper of John Platt in 1996
    - This is the SVM algorithm I implemented in C
- Idea: coordinate descent

SMO for SVM

$$\max_{\alpha} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{s.t.} \quad \sum_{i=1}^{n} \alpha_i y_i = 0, \; 0 \leq \alpha_i \leq C$$

- Coordinate ascent: updating each element individually to reduce the optimization problem to a sequence of low-dim optimization problems
- however, for SVM, this does not work [Why?]

SMO for SVM

- each time optimize w.r.t. a pair of variables and reduce the problem to

$$\begin{aligned} \max_\alpha \quad & W(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y^{(i)} y^{(j)} \alpha_i \alpha_j \langle x^{(i)}, x^{(j)} \rangle. \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C, \quad i = 1, \ldots, m \\ & \sum_{i=1}^{m} \alpha_i y^{(i)} = 0. \end{aligned}$$

$$\alpha_1 y^{(1)} + \alpha_2 y^{(2)} = -\sum_{i=3}^{m} \alpha_i y^{(i)}.$$

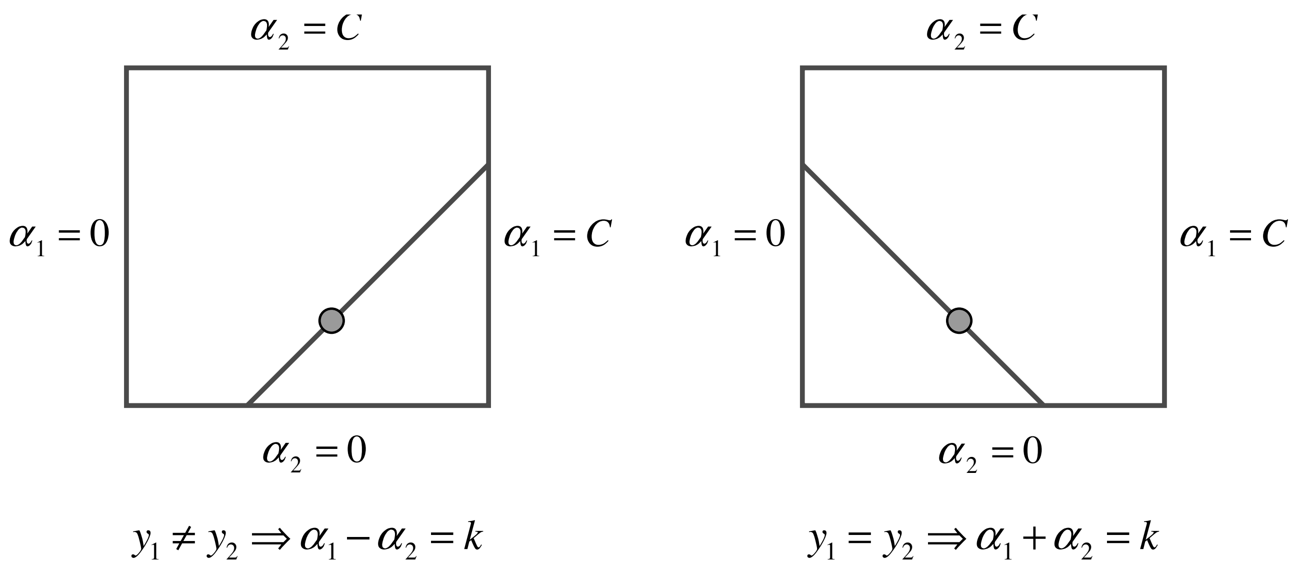
$$\alpha_1 y^{(1)} + \alpha_2 y^{(2)} = \zeta. \qquad \alpha_1 = (\zeta - \alpha_2 y^{(2)}) y^{(1)}.$$

$$W(\alpha_1, \alpha_2, \ldots, \alpha_m) = W((\zeta - \alpha_2 y^{(2)}) y^{(1)}, \alpha_2, \ldots, \alpha_m)$$

SMO for SVM

- Each time minimize a simple quadratic function with two variables and box constraints

$$W(\alpha_1, \alpha_2, \ldots, \alpha_m) = W((\zeta - \alpha_2 y^{(2)}) y^{(1)}, \alpha_2, \ldots, \alpha_m)$$



SMO for SVM

Repeat till convergence {

1. Select some pair α_i and α_j to update next (using a heuristic that tries to pick the two that will allow us to make the biggest progress towards the global maximum).
2. Reoptimize $W(\alpha)$ with respect to α_i and α_j, while holding all the other α_k's $(k \neq i, j)$ fixed.

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SVM solvers

- Many SVM solvers for python and other languages
  - Scikt-learn
  - LibSVM
  - SVM-light
  - SVM-torch
  - Matlab ML toolkit